

5 6 12 13 14 15 16 25 26 27 28 1 2 11 29 30 40 41 42 43 51 52 54 55 56 82 83 84 85 86 87 53 chain bonds : 1-63 1-64 2-9 3-61 3-62 4-59 4-60 5-7 6-8 10-17 10-18 10-12 15-65 19-20 19-24 21-22 21-23 25-68 26-31 42-75 43-72 44-71 45-73 49-50 27-67 28-66 29-70 30-69 31-32 39-41 39-46 40-74 51-79 52-78 53-77 54-76 55-80 86-88 ring bonds 6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-1 27-28 28-29 29-30 40-41 40-45 41-42 42-43 43-44 1-2 1-6 13-14 14-15 15-16 25-26 25-30 26-27 44-45 51-52 51-56 52-53 54-55 82-83 82-87 53~54 55-56 83-84 84-85 85-86 86-87 exact/norm bonds : 1-2 1-6 2-3 2-9 3-4 4-5 5-6 5-7 6-8 10-17 10-18 10-12 19-24 21-23 31-32 39-46 49-50 86-88 exact bonds : 1-63 1-64 3-61 3-62 4-59 4-60 15-65 19-20 21-22 25-68 26-31 27-67 28-66 30-69 39-41 40-74 42-75 29-70 43-72 44-71 45-73 51-79 54-76 55-80 normalized bonds: 11-12 11-16 12-13 13-14 14-15 15~16 25-26 25-30 26-27 27-28 28-29 29-30 40-41 40-45 41-42 42-43 43-44 44-45 51-52 51-56 52-53 53-54 54-55 55-56 82-83 82-87 86-87 83-84 84-85 85-86

G1:[*1],[*2],[*3],[*4],[*5]

89

ring nodes :

G3: [*4], [*6], [*7], [*8], [*9]

G4:[*4],[*6],[*7],[*8],[*9]

Connectivity:

50:1 E exact RC ring/chain 91:1 E exact RC ring/chain Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 39:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:CLASS 49:CLASS 50:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS 82:Atom 83:CLASS 84:CLASS 85:CLASS 86:Atom 87:Atom 88:CLASS 91:CLASS

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FULL SCREEN SEARCH COMPLETED - 214738 TO ITERATE

100.0% PROCESSED 214738 ITERATIONS (1 INCOMPLETE) 6 ANSWERS

SEARCH TIME: 00.00.07

L3 6 SEA SSS FUL L1

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SINCE FILE TOTAL

ENTRY SESSION 148.55 148.76

FULL ESTIMATED COST

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FILE COVERS 1907 - 25 Jul 2003 VOL 139 ISS 5 FILE LAST UPDATED: 24 Jul 2003 (20030724/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4

6 L3

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L4
      ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
      2003:334911 CAPLUS
ΑN
DN
TI
      Preparation of dihydroxypyrimidine carboxamide inhibitors of HIV integrase
      Di Francesco, Maria Emilia; Gardelli, Cristina; Harper, Steven; Matassa,
IN
      Victor Giulio; Muraglia, Ester; Nizi, Emanuela; Pace, Paola; Pacini,
      Barbara; Petrocchi, Alessia; Poma, Marco; Summa, Vincenzo
PA
      Istituto di Ricerche di Biologia Molecolare P. Angeletti S.p.A., Italy
      PCT Int. Appl., 315 pp.
SO
      CODEN: PIXXD2
      Patent
DT
      English
LA
FAN.CNT 1
      PATENT NO.
                            KIND
                                   DATE
                                                      APPLICATION NO.
PΙ
      WO 2003035076
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                NE, SN, TD, TG
PRAI US 2001-348195P
                            P
                                    20011026
os
      MARPAT 138:354000
GI
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$$\begin{array}{c|c}
 & OR^2 \\
 & OH \\
 & R^3 \\
 & N \\
 & R^4 \\
 & O \\
 & I
\end{array}$$

The title 4,5-dihydroxypyrimidine-6-carboxamides [I; R1 = H, alkyl, AB haloalkyl, alkoxy, etc.; R2 = H, alkyl, haloalkyl, hydroxyalkyl, etc.; R3 = H, alkyl; R4 = H, alkyl, haloalkyl, etc.] which are inhibitors of HIV integrase and inhibitors of HIV replication, and therefore are useful in the prevention and treatment of infection by HIV and in the prevention, delay in the onset, and treatment of AIDS, were prepd. Thus, refluxing N-hydroxythiophene-2-carboximidamide with di-Me acetylenedicarboxylate in CHCl3 followed by reacting the resulting Me 5,6-dihydroxy-2-(2thienyl)pyrimidine-4-carboxylate with 4-fluorobenzylamine in DMF afforded I [R1 = 2-thienyl; R2 = H; R3 = 4-FC6H4CH2; R4 = H]. The compds. I are employed against HIV infection and AIDS as compds. per se or in the form of pharmaceutically acceptable salts. The compds. I and their salts can be employed as ingredients in pharmaceutical compns., optionally in combination with other antivirals, immunomodulators, antibiotics or vaccines.

IT 519032-89-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of dihydroxypyrimidine carboxamide inhibitors of HIV integrase)

RN 519032-89-4 CAPLUS

CN 4-Pyrimidinecarboxamide, 2-(1-acetyl-2,4-dimethyl-2-piperazinyl)-N-[(4-fluorophenyl)methyl]-1,6-dihydro-5-hydroxy-6-oxo- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 2002:400770 CAPLUS
- DN 137:382480
- TI Mitochondrial gene rearrangements confirm the parallel evolution of the crab-like form
- AU Morrison, C. L.; Harvey, A. W.; Lavery, S.; Tieu, K.; Huang, Y.; Cunningham, C. W.
- CS Department of Fisheries Science, College of William and Mary, Gloucester Point, VA, 23062, USA
- SO Proceedings of the Royal Society of London, Series B: Biological Sciences (2002), 269(1489), 345-350
 CODEN: PRLBA4; ISSN: 0962-8452
- PB Royal Society
- DT Journal
- LA English
- The repeated appearance of strikingly similar crab-like forms in independent decapod crustacean lineages represents a remarkable case of parallel evolution. Uncertainty surrounding the phylogenetic relationships among crab-like lineages has hampered evolutionary studies. As is often the case, aligned DNA sequences by themselves were unable to fully resolve these relationships. Four nested mitochondrial gene rearrangements-including 1 of the few reported movements of an arthropod protein-coding gene-are congruent with the DNA phylogeny and help to resolve a crucial node. A phylogenetic anal. of DNA sequences, and gene rearrangements, supported 5 independent origins of the crab-like form, and suggests that the evolution of the crab-like form may be irreversible. This result supports the utility of mitochondrial gene rearrangements in phylogenetic reconstruction.
- IT 243866-56-0
 - RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 - (amino acid sequence; mitochondrial gene rearrangements confirm the parallel evolution of the crab-like form)
- RN 243866-56-0 CAPLUS
- CN L-Valine, L-leucyl-L-seryl-L-tryptophyl-L-glutaminyl-L-seryl-L-alanyl-L-leucyl-L-valyl-L-alanyl-L-prolyl-L-leucyl-L-histidyl-L-seryl-L-seryl-L-seryl-L-leucyl-L-seryl-L-isoleucyl-L-phenylalanyl-L-seryl-L-tyrosyl-L-tyrosyl-L-seryl-L-cysteinyl-L-arginyl-L-seryl-L-methionyl-L-phenylalanyl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2001:900136 CAPLUS

DN 137:15276

TI Structure-activity relationships in platelet-activating factor (PAF). 11-From PAF-antagonism to phospholipase A2 inhibition: syntheses and structure-activity relationships in 1-arylsulfamido-2-alkylpiperazines

AU Binisti, Carine; Assogba, Leon; Touboul, Estera; Mounier, Carine; Huet, Jack; Ombetta, Jean-Edouard; Dong, Chang Zhi; Redeuilh, Catherine; Heymans, Francoise; Godfroid, Jean-Jacques

CS Laboratoire de Pharmacochimie Moleculaire, Universite Paris 7-Denis Diderot, Paris, F-75251, Fr.

SO European Journal of Medicinal Chemistry (2001), 36(10), 809-828 CODEN: EJMCA5; ISSN: 0223-5234

PB Editions Scientifiques et Medicales Elsevier

DT Journal

LA English

AB 1-Benzoyl-2-alkyl piperazines are strong inhibitors of Group I and II secreted PLA2s. An improvement of their activity was obtained by replacing the amide function by a sulfamide and by introduction of electro-donor substituents on the para position of the benzenesulfonyl moiety. Neither the position on one of the carbon of the piperazine ring nor the abs. configuration of this carbon have an effect on the affinity for one or the other group of PLA2, but the lipophilicity remains for these series an essential parameter. In addn. structure-activity relationships allow new hypothesis on interaction of these piperazine derivs. with the catalytic site of PLA2s.

IT 433934-45-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structure-activity relationships in platelet-activating factor)

RN 433934-45-3 CAPLUS

CN Piperazine, 4-methyl-1-[(4-methylphenyl)sulfonyl]-2-octyl-,
monohydrochloride (9CI) (CA INDEX NAME)

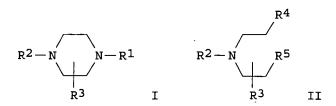
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RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
L4
AN
       2000:756684 CAPLUS
DN
       133:321901
       Novel synthesis of piperazine ring
ΤI
       Dolitzky, Ben-Zion
IN
       Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals Usa,
PA
SO
       PCT Int. Appl., 19 pp.
       CODEN: PIXXD2
       Patent
DT
       English
LA
FAN.CNT 1
       PATENT NO.
                                 KIND DATE
                                                                 APPLICATION NO.
                                                                                          DATE
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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       WO 2000-US9418
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OS
       CASREACT 133:321901; MARPAT 133:321901
GI
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AB A novel process for prepg. the compds I [R1 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy; R2 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy, tosyl, formyl, acetyl, amino; R3 = (un)substituted alkyl, alkoxy, aryl, aryloxy, arylalkoxy], comprising the step of reacting the compd. II [R4, R5 = F, Cl, Br, I] with H2NR1, is disclosed. The compds. I are useful as intermediates in the synthesis of the antidepressant mirtazapine and other tetracyclic compds.

IT 303069-12-7P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel synthesis of piperazine ring)
RN 303069-12-7 CAPLUS
CN Piperazine, 4-methyl-1-[(4-methylphenyl)sulfonyl]-2-phenyl- (9CI) (CA INDEX NAME)

- L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1999:427751 CAPLUS
- DN 131:226345
- TI Mitochondrial Genes Collectively Suggest the Paraphyly of Crustacea with Respect to Insecta
- AU Garcia-Machado, Erik; Pempera, Malgorzata; Dennebouy, Nicole; Oliva-Suarez, Mario; Mounolou, Jean-Claude; Monnerot, Monique
- CS Calle 1ra No. 2808, Centro de Investigaciones Marinas, Universidad de La Habana, C. Habana, Cuba
- SO Journal of Molecular Evolution (1999), 49(1), 142-149 CODEN: JMEVAU; ISSN: 0022-2844
- PB Springer-Verlag New York Inc.
- DT Journal
- LA English
- AB Complete sequences of seven protein coding genes from Penaeus notialis mitochondrial DNA were compared in base compn. and codon usage with homologous genes from Artemia franciscana and four insects. The crustacean genes are significantly less A + T-rich than their counterpart in insects and the pattern of codon usage (ratio of G + C-rich vs. A + T-rich codon) is less biased. A phylogenetic anal. using amino acid sequences of the seven corresponding polypeptides supports a sister-taxon status for mollusks-annelid and arthropods. Furthermore, a distance matrix-based tree and two most-parsimonious trees both suggest that crustaceans are paraphyletic with respect to insects. This is also supported by the inclusion of Panulirus argus COII (complete) and COI and COIII (partial) sequence data. From anal. of single and combined genes to infer phylogenies, it is obsd. that obtained from single genes are not well supported in most topologies cases and notably differ from that of the tree based on all seven genes.
- IT 243866-56-0

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(amino acid sequence; mitochondrial gene sequences suggest paraphyly of crustacea with respect to insecta)

- RN 243866-56-0 CAPLUS
- CN L-Valine, L-leucyl-L-seryl-L-tryptophyl-L-glutaminyl-L-seryl-L-alanyl-L-leucyl-L-valyl-L-alanyl-L-prolyl-L-leucyl-L-histidyl-L-seryl-L-seryl-L-seryl-L-seryl-L-seryl-L-seryl-L-seryl-L-seryl-L-seryl-L-tyrosyl-L-tyrosyl-L-seryl-L-arginyl-L-seryl-L-methionyl-L-phenylalanyl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1969:87746 CAPLUS

DN 70:87746

TI Composition and structure of 2-methylpiperazine-carbon disulfide complex

AU Nishimura, Haruki; Kinugasa, Tomoko

CS Res. Lab., Dainippon Pharm. Co., Ltd., Osaka, Japan

SO Chemical & Pharmaceutical Bulletin (1969), 17(1), 94-7 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

AB 2-Methylpiperazine-CS2 complex, obtained by the reaction of 2-methylpiperazine with CS2, was not 2-methylpiperazine-2-carbodithioic acid, but a mixt. composed of 3-methylpiperazine-1-carbodithioic acid and the 2-methylpiperazine salt of 2-methylpiperazine-1,4-dicarbodithioic acid.

IT 23121-58-6P

RN 23121-58-6 CAPLUS

CN Piperazine, 2,4-dimethyl-1-(p-tolylsulfonyl)-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 46854-82-4 CMF C13 H20 N2 O2 S

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

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